21.49 REGION

REGION specifies the location of materials in a previously defined mesh. Every triangle must be defined as a material.

Syntax

```
REGION NUMBER=<n> <material> [<position>]
```

Parameter	Type	Default	Units
ABS	Logical	False	
A.MAX	Real		degrees
A.MIN	Real		degress
A-SILICO	Logical	False	
ACCEPTORS	Real	0.0	cm^{-3}
ALGAAS	Logical	False	
ALINAS	Logical	False	
ASUB	Real	1.0	Å
BOTTOM	Logical	False	
CALC.STRAIN	Logical	False	
COMPX.BOTTOM	Real	0.0	
COMPY.BOTTOM	Real	0.0	
COMPX.TOP	Real	0.0	
COMPY.TOP	Real	0.0	
CONDUCTOR	Logical	False	
CONVERT	Logical	False	
DEC.C1	Real	0.0	eV
DEC.C2	Real	0.0	eV
DEC.C3	Real	0.0	eV
DEC.D2	Real	0.0	eV
DEC.D4	Real	0.0	eV
DEC.ISO	Real	0.0	eV
DEV.HH	Real	0.0	eV
DEV.LH	Real	0.0	eV

Parameter	Type	Default	Units
DEV.SO	Real	0.0	eV
DEV.ISO	Real	0.0	eV
DIAMOND	Logical	False	
DONORS	Real	0.0	cm^{-3}
ETA.NEGF	Real	0.0066	eV
EQUIL.NEGF	Logical	False	
FIXED.FERMI	Logical	False	
FN.SIS	Logical	False	
HELMHOLTZ	Logical	True	
GAAS	Logical	False	
GAASP	Logical	False	
GERMANIU	Logical	False	
GRAD.12	Real		µm
GRAD.23	Real		mm
GRAD.34	Real		µm
GRAD.41	Real		µm
GRADED	Logical	False	
HGCDTE	Logical	False	
INGAAS	Logical	False	
INAS	Logical	False	
INASP	Logical	False	
INGAP	Logical	False	
INP	Logical	False	
INSULATO	Logical	False	
IX.LOW	Integer	left of structure	
IX.HIGH	Integer	right of structure	
IX.MAX	Integer	right of structure	
IX.MIN	Integer	left of structure	
IY.LOW	Integer	top of structure	

Parameter	Type	Default	Units
IY.HIGH	Integer	bottom of structure	
IY.MAX	Integer	top of structure	
IY.MIN	Integer	bottom of structure	
IZ.HIGH	Real		
IZ.LOW	Real		
IZ.MAX	Integer		
IZ.MIN	Integer		
LED	Logical	False	
MATERIAL	Character		
MODIFY	Logical	False	
NAME	Character		
NA.TOP	Real	0.0	cm^{-3}
ND.TOP	Real	0.0	cm^{-3}
NA.BOTTOM	Real	0.0	cm^{-3}
ND.BOTTOM	Real	0.0	cm^{-3}
NITRIDE	Logical	False	
NUMBER	Integer		
NX	Real	2	
NY	Real	2	
OXIDE	Logical	False	
OXYNITRI	Logical	False	
P1.X	Real		µm
P1.Y	Real		µm
P2.X	Real		µm
P2.Y	Real		µm
P3.X	Real		µm
P3.Y	Real		µm
P4.X	Real		µm
P4.Y	Real		µm

Parameter	Type	Default	Units
PIEZOELECTRIC	Logical	False	
PIEZO.SCALE	Real	1.0	
POLAR.CHARGE	Real	0.0	cm^{-2}
POLAR.SCALE	Real	1.0	
POLARIZATION	Logical	False	
POLYSILICON	Logical	False	
PSP.SCALE	Real	1.0	
QTREGION	Integer	0	
QWELL	Logical	False	
QWNUM	Integer	-1	
R.MAX	Real		µm
R.MIN	Real		µm
S.OXIDE	Logical	False	
SAPPHIRE	Logical	False	
SCHRO	Logical	True	
SEMICOND	Logical	False	
SELF	Logical	False	
SI3N4	Logical	False	
SIC	Logical	False	
SIGE	Logical	False	
SILICON	Logical	False	
SIO2	Logical	False	
STAY	Logical	False	
STRAIN	Real	0.0	
STR.BOT	Real	0.0	
STR.TOP	Real	0.0	
SUBSTRATE	Logical	False	
SX	Real	0.0	
SY	Real	0.0	

Parameter	Type	Default	Units
THICKNESS	Real	0.0	µm
TOP	Logical	False	
TRAPPY	Logical	False	
USER.GROUP	Character		
USER.MATERIAL	Character		
WELL.CNBS	Integer	1	
WELL.DEBUG	Logical	False	
WELL.FIELD	Logical	True	
WELL.GAIN	Real	1.0	
WELL.NX	Integer	10	
WELL.NY	Integer	10	
WELL.NZ	Integer	10	
WELL.OVERLAP	Real		
WELL.VNBS	Integer	1	
X.COMP	Real	0.0	
X.MAX	Real	right of structure	µm
X.MIN	Real	left of structure	µm
X.MOLE	Real	0.0	
Y.MOLE	Real	0.0	
Y.COMP	Real	0.0	
Y.MIN	Real	top of structure	µm
Y.MAX	Real	bottom of structure	µm
Z.MAX	Real		
Z.MIN	Real		
ZEROBP	Logical	False	
ZNSE	Logical	False	
ZNTE	Logical	False	

Description

n	Specifies a region number from 1 to 200.
material	This is one or more of the material names described below.
position	This is one or more of the position parameters described below.

Material Parameters

ABS	Specifies that quantum confinement is included in the calculation of absorption or imaginary index of refraction. To use this model, you must also specify QWELL on the REGION statement. See Section 10.8.3 "Quantum Well Absorption".
ACCEPTORS	Specifies a uniform density of ionized acceptors in the region.
ASUB	Specifies the substrate lattice constant for strain calculations as described in Section 3.6.11 "Epitaxial Strain Tensor Calculation in Wurtzite".
CALC.STRAIN	Specifies that the strain in the region is calculated from the lattice mismatch with adjacent regions.
COMPX.BOTTOM **COMPY.BOTTOM** **COMPX.TOP** **COMPY.TOP**	Specify the composition fractions at the top and bottom of a region when linearly graded. Linear grading is specified by the GRADED parameter. See Section 2.6.4 "Automatic Meshing (Auto-meshing) Using The Command Language".
CONDUCTOR	Specifies that the region is to be simulated as a conductor. This means that the conduction equation is solved for the region.
CONVERT	This is an alias for MODIFY.
DEC.C1	This is a conduction band shift for 1st pair of electron valleys.
DEC.C2	This is a conduction band shift for 2nd pair of electron valleys.
DEC.C3	This is a conduction band shift for 3rd pair of electron valleys.
DEC.D2	This is a conduction band shift for Δ2 electron valleys if DEC.C1 is not set.
DEC.D4	This is a conduction band shift for Δ4 electronvalleys if DEC.C2 is not set.
DEC.ISO	This is a conduction band shift for isotropic electron band, when NUM.DIRECT=1.
DEV.HH	This is a valence band shift for heavy holes.
DEV.LH	This is a valence band shift for light holes.
DEV.ISO	This is a valence band shift for isotropic hole band, when NUM.BAND=1.
DEV.SO	This is a valence band shift for split-off holes.

DONORS	Specifies a uniform density of ionized donors in the region.
ETA.NEGF	An imaginary optical potential, added to Hamiltonian of quasi-equilibrium regions in planar NEGF model.
EQUIL.NEGF	Specified that the region will be trated as quasi-equilibrium in planar NEGF model.
GRAD.<n>	Specifies the compositional gradings for heterojunctions along each side of the region rectangle or quadrilateral. The value of the GRAD parameters specifies the distance at which the composition fraction reduces to zero. A value of 0.0 specifies that the heterojunction is abrupt. The value of <n> can be the numbers: 12, 23, 34, and 41. The meanings of these numbers is down below. • 12 = top surface • 23= right hand side • 34= bottom surface • 41 = left hand side These correspond to the point indices around the rectangular region working clockwise from top left.
GRADED	Specifies that the region has linear compositional or doping variation or both. See also COMPX.BOTTOM, COMPY.BOTTOM, COMPX.TOP, COMPY.TOP, ND.BOTTOM, ND.TOP, NA.BOTTOM and NA.TOP.
HELMHOLTZ	Allows (default) or prevents a solution of vector Helmholtz equation in the region.
LED	Specifies that the region is to be treated as a light emitting region and included in postprocessing for LED analysis. See Chapter 11 "LED: Light Emitting Diode Simulator".
MATERIAL	Specifies the material used for the region. Valid material names are listed in Table B-1. All materials are divided into three classes: semiconductors, insulators and conductors.

Note: You can specify the following logical parameters to indicate the region material instead of assigning the MATERIAL parameter: SILICON, GAAS, POLYSILI, GERMANIU, SIC, SEMICOND, SIGE, ALGAAS, A-SILICO, DIAMOND, HGCDTE, INAS, INGAAS, INP, S.OXIDE, ZNSE, ZNTE, ALINAS, GAASP, INGAP, INASP, OXIDE, SIO2, NITRIDE, SI3N4, INSULATO, SAPPHIRE, and OXYNITRI.

MODIFY	This is used to modify the characteristics of regions imported into the simulator. See Section 2.6.5 "Modifying Imported Regions". The alias for this parameter is CONVERT.
NAME	Specifies the name of the region. The name can be used in the MODELS, MATERIAL, and IMPACT statements to provide regionally dependent models. This name is just a label. It doesn't imply any material parameter settings.
ND.BOTTOM **ND.TOP** **NA.BOTTOM** **NA.TOP**	Specify the doping concentrations at the top and bottom of a region when linearly graded. Linear grading is specified by the GRADED parameter. See Section 2.6.4 "Automatic Meshing (Auto-meshing) Using The Command Language".
NUMBER	Assigns a region number. Multiple REGION lines with the same number can be used to define region shapes made from several rectangles.
PIEZO.SCALE	This is an alias for POLAR.SCALE.
PIEZOELECTRIC	This is an alias for POLARIZATION.
POLARIZATION	Enables the automatic calculation of added interface charge due to spontaneous and piezoelectric polarization. The alias for this parameter is PIEZOELECTRIC. See Section 3.6.12 "Polarization in Wurtzite Materials".
POLAR.CHARGE	Specifies polarization charge densities to replace the density calculated using Equations 3-575 and 3-576.
POLAR.SCALE	Specifies a constant scale factor multiplied by the calculated spontaneous and piezoelectric polarization charges when you enable polarization by setting the POLARIZATION parameter of the REGION statement. The alias for this parameter is PIEZO.SCALE. See Section 3.6.12 "Polarization in Wurtzite Materials".
PSP.SCALE	Specifies a constant scale factor similar to POLAR.SCALE but applied only to spontaneous polarization.
QTREGION	This designates the region as a quantum barrier for the quantum barrier tunnelling models SIS.EL and SIS.HO. The index of the QTREGION is also set with this parameter. For further information, see Section 5.2.4 "Non-local Quantum Barrier Tunneling Model".
QWELL	Specifies that the region is treated as a quantum well for calculation of radiative recombination or gain or both for certain optoelectronic models.
QWNUM	Optionally sets the number of the quantum well region.
SCHRO	Allows (default) or prevents a solution of Schrodinger in the region. Switch it off, if the region is to be treated classically.

STRAIN	Specifies the strain in the region. (Negative strain is compressive).
STR.BOT **STR.TOP**	Specify the strain at the bottom and top of the region for calculations of the k.p model. The strain values between the top and bottom of the region are linearly interpolated.
SUBSTRATE	This is a logical parameter indicating that the specified region should be considered as the the substrate for strain calculations as described in Section 3.6.11 "Epitaxial Strain Tensor Calculation in Wurtzite".
TRAPPY	Used only with the BESONOS model. This indicates that a Silicon-Nitride region will be able to trap electrons and holes.
USER.GROUP	Specifies the material group for the user-defined material. USER.GROUP can be either SEMICONDUCTOR, INSULATOR, or CONDUCTOR.
USER.MATERIAL	Specifies a user-defined material name. The specified material name can be any name except that of a default material, such as Silicon. You should define each material with an accompanying definition in the MATERIAL statement. You can define up to 50 user-defined materials.
WELL.CNBS **WELL.VNBS**	Specify the number of bound states retained for calculation of radiative recombination or gain if the region is treated as a quantum well as specified by the QWELL parameter.
WELL.FIELD	Specifies that the calculations of bound state energies should include the effects of the local field.
WELL.GAIN	Specifies a constant scale factor multiplied by the calculated gain to give the net gain used for certain optoelectronic calculations.
WELL.NX **WELL.NY** **WELL.NZ**	Specifies the number of grid points in x, y, and z directions for Schrodinger equation in a quantum well region.
WELL.OVERLAP	Specifies the wavefunction overlap integral. If WELL.OVERLAP is not specified, then the overlap integral is calculated from the wavefunctions.

Note: The highest region number takes precedence if REGION definitions overlap.

ZEROBQP	Specifies that in the given region the Bohm quantum potential is not solved and is assigned to zero.

Position Parameters

You can use grid indices to define a region only when the mesh is rectangular. To define a region with a rectangular mesh, use the X.MESH and Y.MESH statements to specify grid indices.

You can also use the IX.HIGH, IX.LOW, IY.HIGH, and IY.LOW parameters to specify x and y mesh line number values.

Note: To add regions to irregular meshes, such as those from ATHENA, specify the boundaries with the X.MAX, X.MIN, Y.MAX, and Y.MIN parameters.

A.MAX	Specifies the maximum angle of a 3D cylindrical region.
A.MIN	Specifies the minimum angle of a 3D cylindrical region.
BOTTOM	Specifies that the region is to be added at the bottom (starting at the maximum previously specified Y coordinate and extending in the positive Y direction) of the structure.
FN.SIS	Applies to the Fowler-Nordheim model for an interface to the insulator region having this attribute. Any Fowler-Nordheim current being evaluated is not assigned to a contact. Instead, it is assumed to pass from one semiconductor region to another through the tagged region.
IX.HIGH	Specifies the maximum x value of the grid index. The alias for this parameter is IX.MAX.
IX.LOW	Specifies the minimum x value of the grid index. The alias for this parameter is IX.MIN.
IY.HIGH	Specifies the maximum y value of the grid index. The alias for this parameter is IY.MAX.
IY.LOW	Specifies the minimum y value of the grid index. The alias for this parameter is IY.MIN.
IZ.HIGH	Specifies the maximum z value of the grid index. The alias for this parameter is IZ.MAX.
IZ.LOW	Specifies the minimum z value of the grid index. The alias for this parameter is IZ.MIN.
IX.MAX **IX.MIN** **IY.MAX** **IY.MIN** **IZ.MAX** **IZ.MIN**	These are aliases for IX.HIGH, IX.LOW, IY.HIGH, IY.LOW, IZ.HIGH, and IY.LOW.
NX	Specifies the number of uniformly spaced mesh lines to be added to resolve the region in the X direction.
NY	Specifies the number of uniformly spaced mesh lines to be added to resolve the region in the Y direction.

STAY	This is used in automeshing to create material variations in the X direction. See Section 2.6.4 "Automatic Meshing (Auto-meshing) Using The Command Language".
SX	Specifies the spacing between mesh lines to be applied at the edges of the region in the X direction.
SY	Specifies the spacing between mesh lines to be applied at the edges of the region in the Y direction.
P1.X	X coordinate of 1st corner of REGION.
P1.Y	Y coordinate of 1st corner of REGION.
P2.X	X coordinate of 2nd corner of REGION.
P2.Y	Y coordinate of 2nd corner of REGION.
P3.X	X coordinate of 3rd corner of REGION.
P3.Y	Y coordinate of 3rd corner of REGION.
P4.X	X coordinate of the last corner of REGION.
P4.Y	Y coordinate of the last corner of REGION.
THICKNESS	Specifies the thickness of the region in the Y direction. This parameter must accompany the specification of the TOP or BOTTOM parameters.
TOP	Specifies that the region is to be added at the top (starting at the minimum previously specified Y coordinate and extending in the negative Y direction) of the structure.
R.MAX	Specifies the maximum radius of a 3D cylindrical region.
R.MIN	Specifies the minimum radius of a 3D cylindrical region.
X.MAX	Specifies the maximum x-boundary.
X.MIN	Specifies the minimum x-boundary.
X.COMP, X.MOLE	This is the composition fraction (X) for a region with a composition dependent cations (e.g., AlGaAs).
Y.COMP, Y.MOLE	This is the composition fraction (Y) for a region with a composition dependent anions(e.g., InGaAsP).
Y.MAX	Specifies the maximum y-boundary.
Y.MIN	Specifies the minimum x-boundary.
Z.MIN	Specifies the minimum z-boundary.
Z.MAX	Specifies the maximum z-boundary.

Grid Indices Example

Define a silicon region extending from nodes 1 to 25 in the X direction and from nodes 1 to 20 in the Y direction.

```
REGION NUM=1 IX.LO=1 IX.HI=25 IY.LO= 1 IY.HI=20 MATERIAL=SILICON
```

Non-Rectangular Region Example

Define a region that's composed of two separate rectangular areas. Note that REGION statements are cumulative.

```
REGION NUM=1 IX.LO=4 IX.HI=5 IY.LO=1 IY.HI=20 MATERIAL=OXIDE
REGION NUM=1 IX.LO=1 IX.HI=30 IY.LO=1 IY.HI=37 MATERIAL=OXIDE
```

Typical MOS Example

Define regions for a typical MOS structure.

```
REGION NUM=1 Y.MAX=0 MATERIAL=OXIDE
REGION NUM=2 Y.MIN=0 MATERIAL=SILICON
```

3D Region Definition Example

Define a cube of oxide within a region silicon in 3D.

```
REGION NUM=1 MATERIAL=SILICON
REGION NUM=2 Y.MAX=0.5 X.MIN=0.5 \
X.MAX=1.0 Z.MIN=0.5 Z.MAX=1.0 MATERIAL = OXIDE
```

Graded Heterojunction Definition Example

Define a graded heterojunction of AlGaAs/GaAs.

```
REGION NUM=1 MATERIAL=GaAs Y.MIN=1
REGION NUM=2 MATERIAL=AlGaAs Y.MAX=0.9 X.COMP=0.2 GRAD.34=0.1
```

In this case, the area between y=0.9 and 1.0 is graded in composition from 0.2 to 0.0. The Y.MAX parameter refers to the bottom of the uniform composition region. The actual bottom of the AlGaAs region is Y.MAX+GRAD.34.

Graded x.comp and y.comp Material Definition Example

Define a graded x.comp and y.comp region in ATLAS using the compx.top, compx.bottom, compy.top, and the compy.bottom keywords on the REGION statement. The following example shows the use of compx.top, compx.bottom functions. Similar use, however, can be made of the compy.top and compy.bottom keywords.

You can use the following code to create a graded x.comp AlGaAs region where the x.comp falls off linearly in value from 0.4 to 0.2 from the top of the region to the bottom of the region.

```
region num=1 material=algaas compx.top=0.4 compx.bottom=0.1
```